(Z)-Styrylthioacetic acid

Inchi: InChI=1S/C10H10O2S/c11-10(12)8-13-7-6-9-4-2-1-3-5-9/h1-7H,8H2,(H,11,12)/b7-6-
InchiKey: IUEVBKDVPSQVLM-SREVYHEPSA-N
Formula: C10H10O2S
SMILES: O=C(O)CSC=Cc1ccccc1
Mol. weight [g/mol]: 194.25
CAS: 1914-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-6.67	kJ/mol	Joback Method
hf	-118.92	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	70.33	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.475		Crippen Method
mcvol	147.490	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
tb	673.87	K	Joback Method
tc	898.51	K	Joback Method
tf	368.95	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.85	J/mol×K	673.87	Joback Method
cpg	363.20	J/mol×K	711.31	Joback Method
cpg	372.76	J/mol×K	748.75	Joback Method
cpg	381.60	J/mol×K	786.19	Joback Method
cpg	389.75	J/mol×K	823.63	Joback Method
cpg	397.27	J/mol×K	861.07	Joback Method
cpg	404.20	J/mol×K	898.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1914610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume